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APPLICATION OF THE UNIFAC-CI MODELS FOR PHASE EQUILIBRIA PREDICTIONS OF ORGANIC CHEMICAL SYSTEMS

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Prediction of properties is important in chemical process-product design. Reliable property models are needed for increasingly complex and wider range of chemicals. Group-contribution (GC) methods provide a useful tool but there is a need to validate them and improve their accuracy when complex chemicals are present in the mixtures. In accordance with that, a combined GC and atom connectivity approach that is able to extend the application range of property models has been developed for mixture properties [1,2,3]. This so-called GC^{Plus} approach is a hybrid model which combines GC and molecular descriptor theories such as connectivity indices. Connectivity indices (CI) are formalisms defined via graph theoretical concepts intended to describe the topological characteristics of molecular structures. The main idea is the use of connectivity indices to describe the molecular fragmentation that relates properties which are the molecular interactions with the molecular structures. One established GC method is the UNIFAC model, used to predict activity coefficients for mixtures. The values required for the group interaction parameters (GIPs) are obtained by fitting phase equilibrium data. There are, however many gaps in the UNIFAC parameter table due to lack of data. Alternative to performing measurements, which may be time consuming and not always feasible, values of the missing GIPs, can be predicted through the GC^{Plus} approach and used in the UNIFAC model to calculate activity coefficients. In this work, the application of this hybrid model, called UNIFAC-CI, is highlighted in two industrial case studies. The first one involves pharmaceutical systems where the solubility of complex drug-like molecules in different solvents are investigated. The second case study involves lipid systems where the phase equilibria of a multicomponent system in the deodorization process of oil and fats which also include extraction and refining of high-value commercial by-products are investigated. In each case study, a parameter table that contains all the needed fine tuned binary interaction parameters is developed. In addition, other interesting examples of systems involving the application of the hybrid model will be presented.

References

[1] González, H.E., Abildskov, J., Gani, R., Rosseaux, P., Le Bert, B., “A Method for Prediction of UNIFAC Group Interaction Parameters”, AIChE J., Vol. 53, No. 6, (2007), pp. 1393–1634.
[2] González, H.E., Abildskov, J., Gani, R., “A Computer Aided Framework for Prediction of Properties of Organic Systems”, Fluid Phase Equilibr., (2007), Vol. 261, pp. 199–204.
[3] Mustaffa, A.A., Kontogeorgis, G.M., Gani, R., “Analysis and Application of GC^{Plus} Models for Property Prediction of Organic Chemical Systems”, Fluid Phase Equilibr., (2011), Vol. 302. pp. 274-283.

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